

SUPPORTING INFORMATION

Title: Muriceanol, a 24(28)-Epoxide Sterol Link in the Carbon Flux Toward Side-Chain Dealkylation of Sterols

Author(s): Manuel Lorenzo, Mercedes Cueto, Luis D’Croz, Juan L. Maté, Aurelio San-Martín, José Darías*

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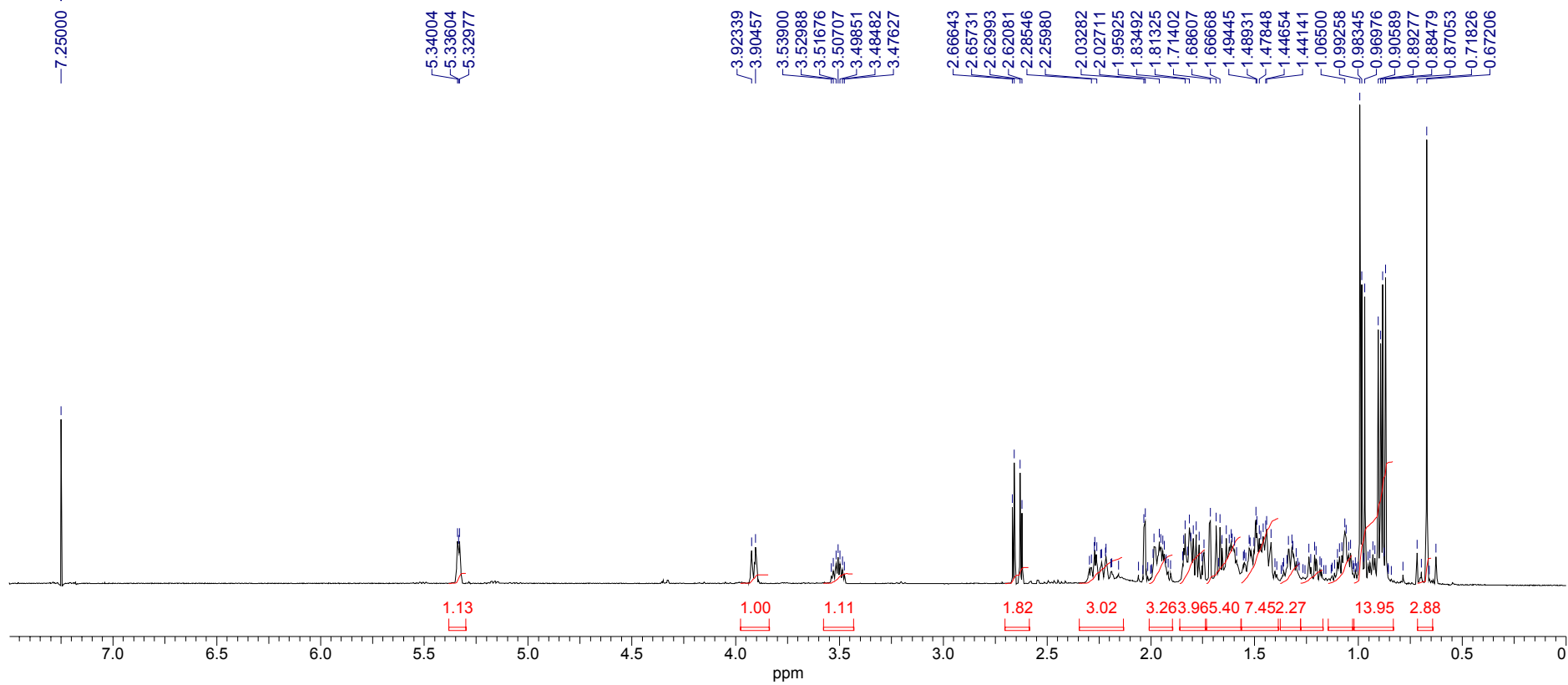
Experimental Section

General Remarks: Optical rotations were measured on a Perkin-Elmer model 343 Plus polarimeter using a Na lamp at 25 °C. IR spectra were obtained with a Perkin-Elmer 1650/FTIR spectrometer. ^1H NMR and ^{13}C NMR, HSQC, HMBC, COSY and NOESY spectra were measured employing a Bruker AMX 500 instrument operating at 500 MHz for ^1H NMR and at 125 MHz for ^{13}C NMR. Two-dimensional NMR spectra were obtained with the standard Bruker software. EIMS and HRMS data were taken on a Micromass Autospec spectrometer. HPLC separations were performed with a Hewlett Packard 1050 (Jaigel-Sil semipreparative column, 10 μ , 20 \times 250 mm) with hexane-EtOAc mixtures. The gel filtration column (Sephadex LH-20) used hexane-MeOH-CH₂Cl₂ (3:1:1) as solvent. The spray reagent for TLC was H₂SO₄-H₂O-AcOH (1:4:20).

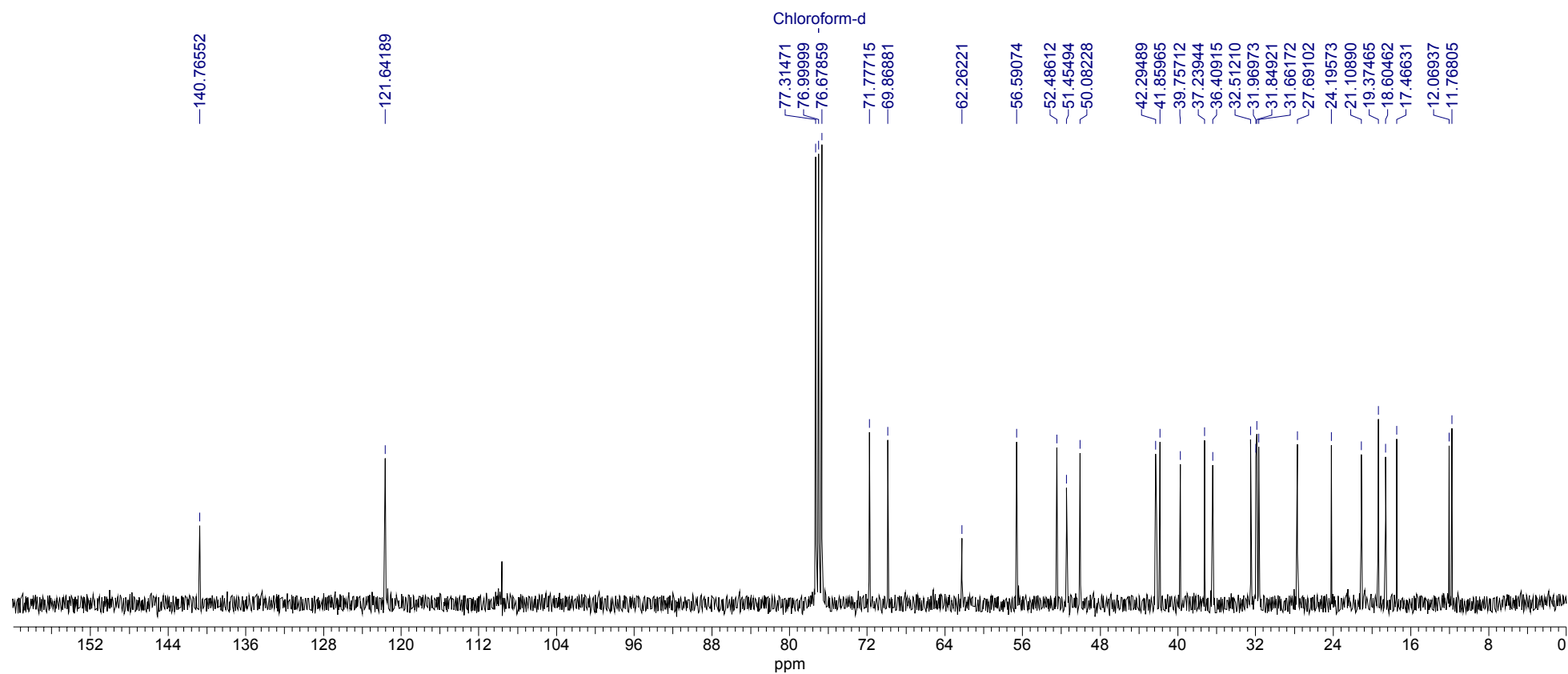
Molecular mechanics: Molecular mechanics calculations was performed using PCMODEL. The force field MMX was employed and the molecules were optimized within the RHF formalism performing a full self-consistent-field (SCF) process. Dielectric constant: 1.5.

^1H NMR of muriceanol 1 in CDCl_3

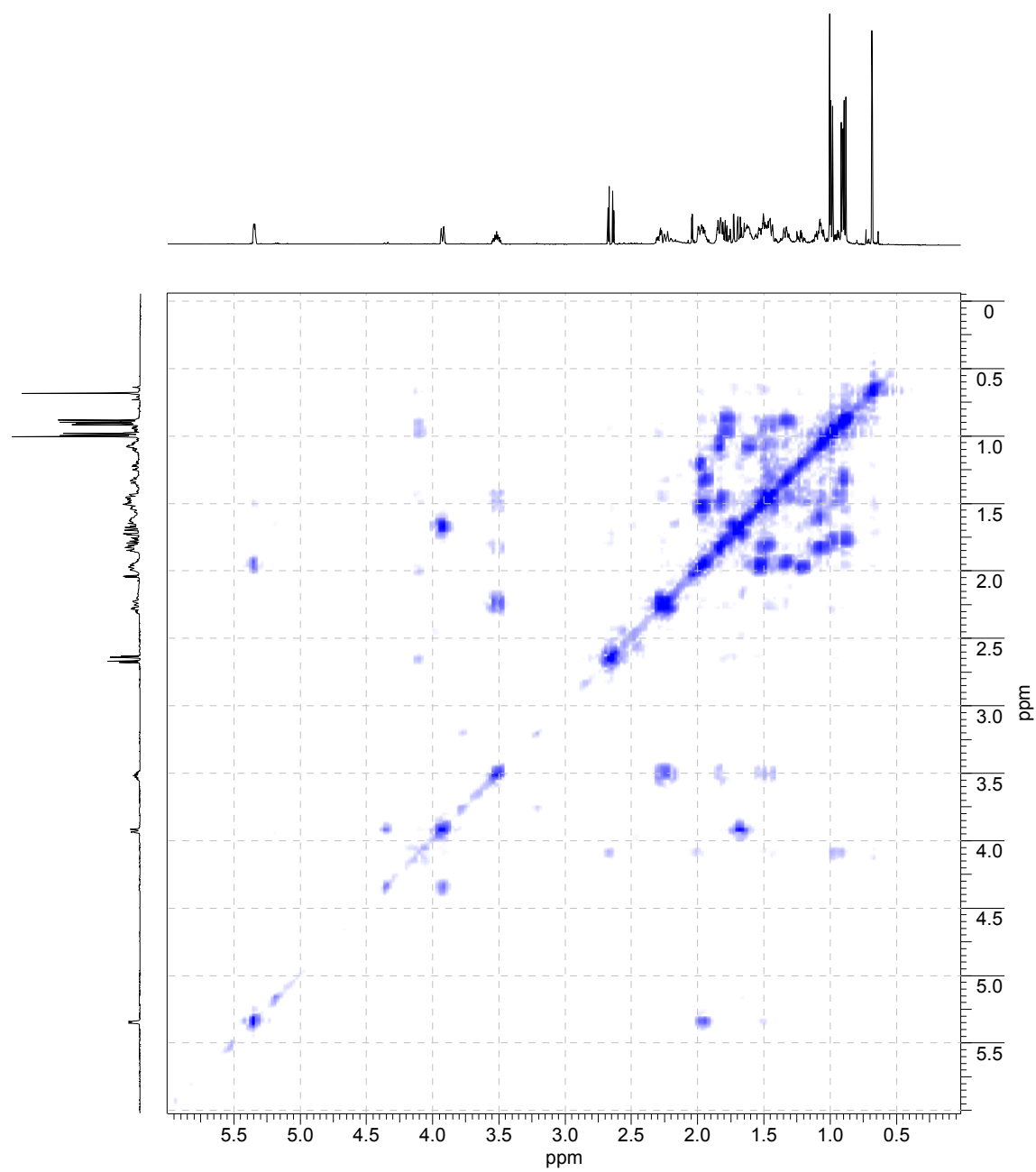
Chloroform-d



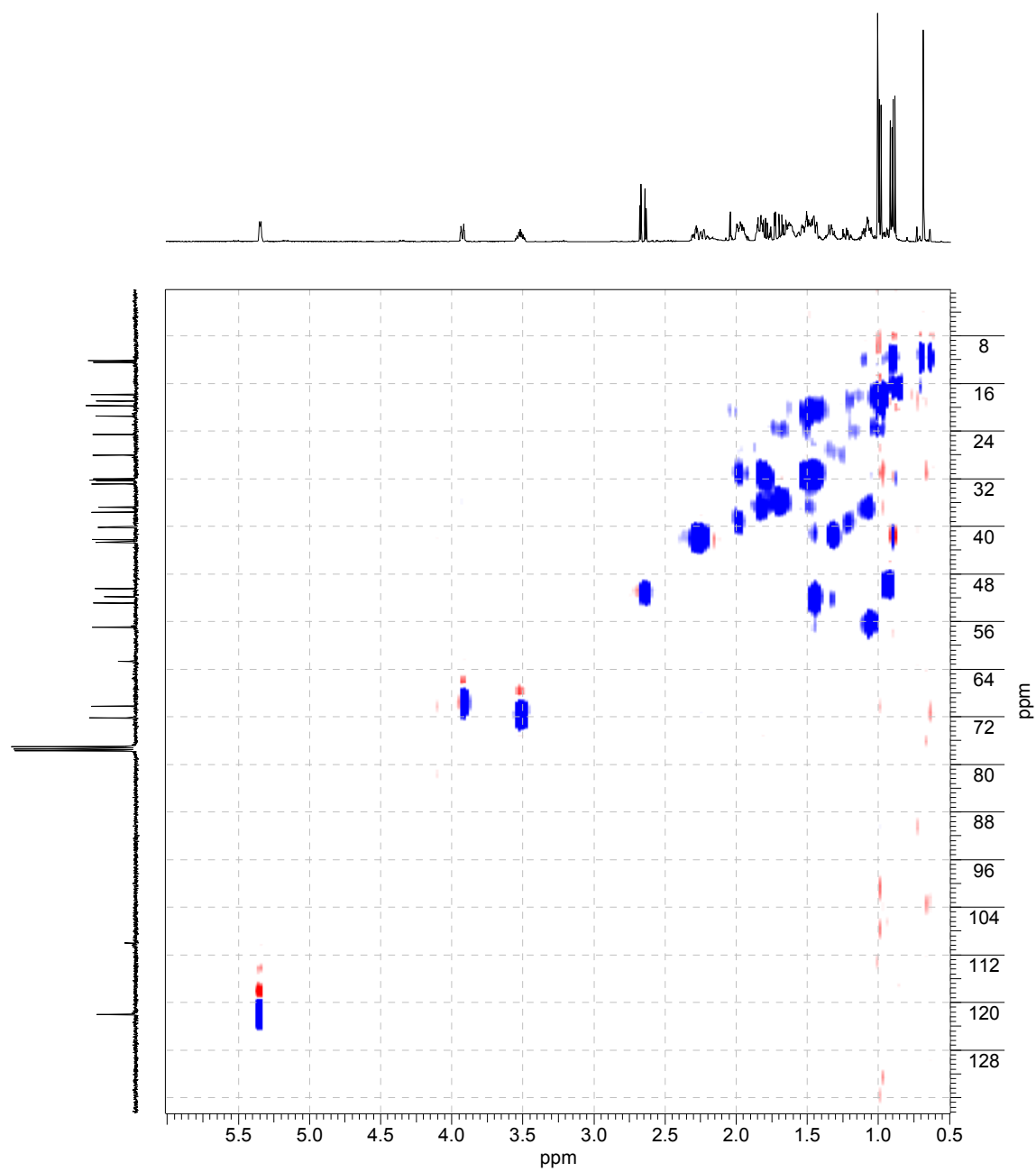
^{13}C NMR of muriceanol 1 in CDCl_3



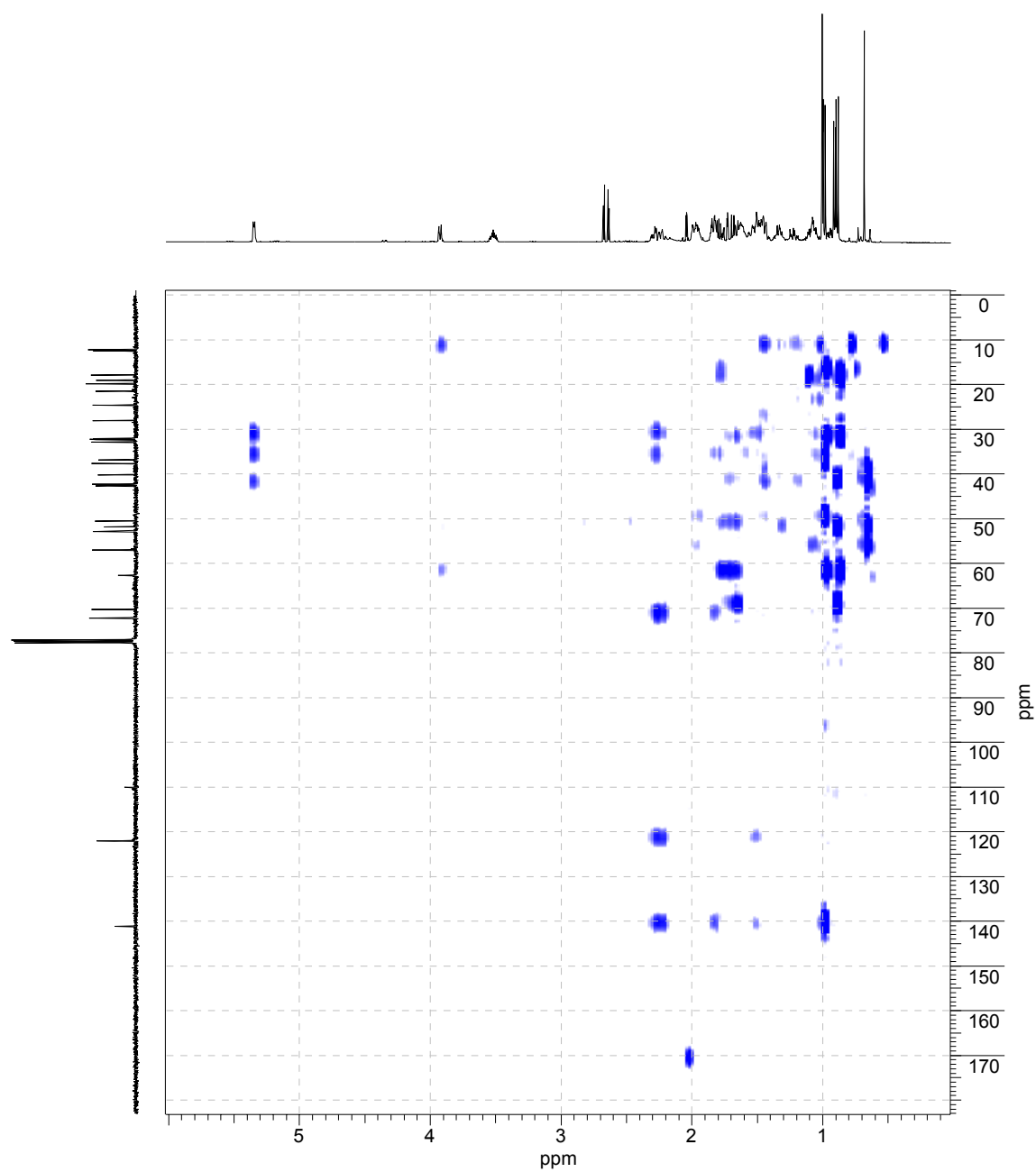
COSY of muriceanol 1 in CDCl₃



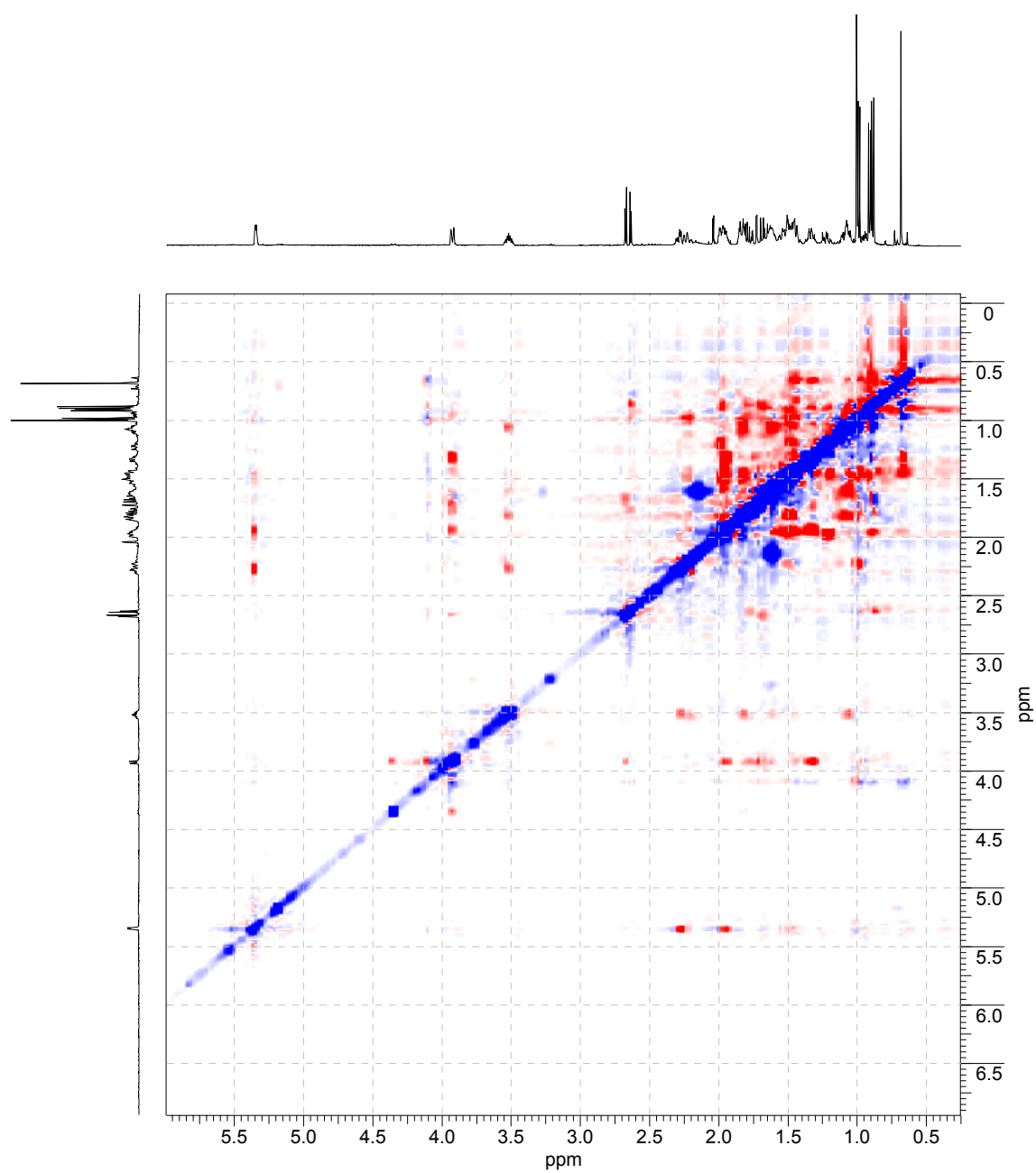
HSQC of muriceanol 1 in CDCl₃



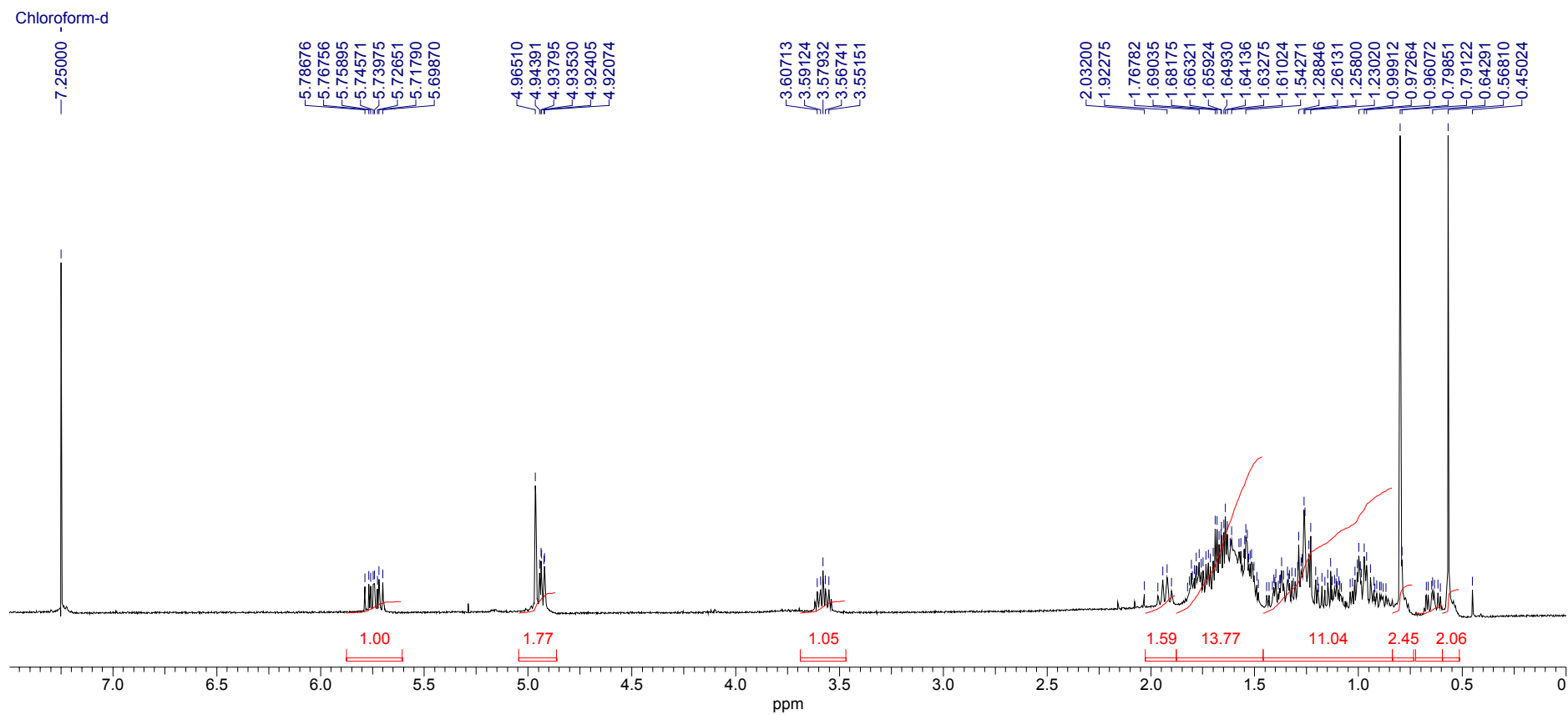
HMBC of muriceanol 1 in CDCl₃



NOESY of muriceanol 1 in CDCl_3



^1H NMR of 2 in CDCl_3



^{13}C NMR of 2 in CDCl_3

